2,2-Dimethylpropane-1,3-diol

126-30-7 | DTXSID8027036

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.294

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 5.71e-01

Nearest Neighbors from the Training Set

Image not found
2,3-Butanediol
Measured: -0.920
Predicted: -0.560

Image not found
2-Ethyl-2-(hydroxymethyl)-1,3-
propanediol
Measured: -1.48
Predicted: -1.17

Image not found
trans-1,2-Cyclohexanediol
Measured: 0.08
Predicted: 2.27e-01

Image not found
2-Methylpropane-1,3-diol
Measured: 0.24
Predicted: -0.254